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Quantum-Mechanical Tunnelling and the Renormalization Group

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Abstract

We explore the applicability of the exact renormalization group to the study of tunnelling phenomena. We investigate quantum-mechanical systems whose energy eigenstates are affected significantly by tunnelling through a barrier in the potential. Within the approximation of the derivative expansion, we find that the exact renormalization group predicts the correct qualitative behaviour for the lowest energy eigenvalues. However, quantitative accuracy is achieved only for potentials with small barriers. For large barriers, the use of alternative methods, such as saddle-point expansions, can provide quantitative accuracy.

Introduction: The exact renormalization group [1, 2] is a powerful method with a wide range of applications in various fields. It provides a framework in which it is possible to study non-perturbative aspects of physical phenomena. This is made possible by an exact renormalization-group equation [2, 3, 4] that describes the dependence of generating functionals for the correlation functions of the theory on a coarse-graining scale. In particular formulations, such as the effective average action [5, 6], an exact equation can be obtained for the flow of the coarse-grained free energy of the system, a quantity with intuitive physical interpretation.

The biggest difficulty one faces in this approach concerns the approximations that must be made in order to turn the exact renormalization-group equation, a functional differential equation, into evolution equations for quantities such as the effective potential. A widely used approximation method employs an expansion of the effective action in the number of derivatives of the fields appearing in it. Its validity, at the formal and practical level, has been studied and tested extensively [6]–[9]. The absence of a small expansion parameter makes the precision of a given truncation in the number of derivatives hard to estimate, and one often must rely on comparisons with alternative methods. However, one can obtain answers for quantities that are difficult to compute, such as critical exponents, amplitudes and the critical equation of state for second-order phase transitions, or the bubble-nucleation rate beyond the semiclassical level for first-order phase transitions [6].

In this letter we are interested in the applicability of the approach to tunnelling phenomena. We work within the formulation of the effective average action [5, 6]. Recent work [10, 11] has demonstrated how the presence of a coarse-graining scale leads to a consistent quantitative description of such phenomena, even beyond the leading semiclassical level. Of related interest is the question of the convexity of the effective potential in field theory, which is induced by tunnelling configurations. This issue has been addressed within the renormalization-group approach as well [12].

The study of the above problems within field theory is often obscured by technical difficulties, such as the need to regulate the ultraviolet divergences, or possible infrared problems arising from the presence of massless modes in the phase with spontaneous symmetry breaking. A much simpler framework is provided by quantum mechanics. One does not have to deal with ultraviolet problems and spontaneous symmetry breaking does not arise. Moreover, the exact answers are well known and comparisons are straightforward. A recent study [13] has also explored the issues we address in this letter. However, it employed an expansion in powers of the field, an approximation that has a significant effect on the results. Our treatment goes beyond this approximation and leads to a more complete conceptual understanding.

The problem: We would like to understand how well quantum-mechanical tunnelling is described by the exact renormalization-group approach. This approach employs field-theoretical language. However, a theory of a real scale field in one time and zero space dimensions can be viewed as a quantum-mechanical system. This mapping is obvious in the functional integral formulation [14] through the replacement of the field ϕ by the position x of the quantum-mechanical particle. As a result, approximations employed in the study of field theories in more than one space-time dimensions can be checked through comparison with exact results in one dimension.

We employ the formalism of the effective average action Γ_k [5, 6] that can be interpreted as a coarse-grained free energy. All fluctuations of the system with characteristic momenta larger than an infrared cutoff k (and wavelengths less than $2\pi/k$) are integrated out and incorporated in the effective couplings appearing in Γ_k. The dependence of Γ_k on the coarse-graining scale k is described by an exact renormalization-group equation [4]. An expansion in derivatives of ϕ results in evolution equations for the functions multiplying the various terms in Γ_k. These form an infinite system of coupled partial

differential equations in ϕ and k. In practice one must truncate this system, by keeping only a finite number of terms in the action.

In one Euclidean space-time dimension, the lowest truncation level (often referred to as the local potential approximation) uses an action of the form[1]

$$\Gamma_k = \int_{-\infty}^{\infty} dt \left\{ \frac{1}{2} \left(\frac{d\phi}{dt} \right)^2 + U_k(\phi) \right\}. \tag{1}$$

At the next level the derivative term is multiplied by a non-trival wavefunction renormalization $Z_k(\phi)$, while higher levels include more derivatives of the field. For the approximation of eq. (1), the exact-renormalization group equation for Γ_k results in the evolution equation [6, 13]

$$\frac{\partial U_k(\phi)}{\partial k} = -\frac{1}{2\pi} \log \left(1 + \frac{1}{k^2} \frac{\partial^2 U_k}{\partial \phi^2} \right) \tag{2}$$

for $U_k(\phi)$. This equation has been derived for a sharp infrared cutoff k that acts like a θ-function, completely integrating out fluctuations of ϕ with momenta $q \geq k$ and excluding fluctuations with $q < k$. It also appears in other formulations of the exact renormalization group in the sharp-cutoff limit [3, 8, 13].

In ref. [13] $U_k(\phi)$ is further expanded in powers of ϕ, and eq. (2) is turned into a system of ordinary differential equations for the coefficients of the expansion. This infinite system is truncated at a finite level. In ref. [12] it was shown that such a truncation does not reproduce correctly the solution of eq. (2) in the regime that is relevant for the convexity of the effective potential. For this reason, we do not make this additional approximation here, but solve numerically the full partial differential equation (2) instead. For this we employ numerical algorithms discussed in ref. [15].

The boundary conditions for the solution of eq. (2) are fixed at a scale $k = \Lambda$ much larger than the physical scales of the low-energy theory. At this "microscopic" level, the potential is determined by the fundamental theory. The case of one dimension is particular in this respect, because the contribution of the ultraviolet regime to the evolution of the potential is negligible. This reflects the absence of ultraviolet divergences in quantum mechanics. As a result, one can interpret the initial condition U_Λ as the potential at the level where no fluctuations of the system are taken into account, i.e. the classical potential V. The solution of eq. (2) in the limit $k \to 0$ incorporates the effect of fluctuations at all scales, and U_0 becomes the effective potential U. In quantum-mechanical terms, U determines the expectation value of the energy of the system for a given expectation value of the position.

We consider Z_2-symmetric classical potentials of the form

$$U_\Lambda = V = -\frac{1}{2} m^2 \phi^2 + \lambda \phi^4 + \frac{m^2}{16\lambda}. \tag{3}$$

Their minima satisfy $U(\phi_{\min}) = 0$. By expressing all dimensionful quantities in units of m, we can set $m = 1$ in the above relation. The presence of a barrier implies that tunnelling configurations can be relevant for this system. For $\lambda \to 0$ the height of the barrier becomes much larger than the distance between the minima and the origin, and we expect tunnelling to play an important role.

The solution: Starting with the above initial condition, we solve the partial differential equation (2) numerically. A typical solution is presented in fig. 1 for $\lambda = 0.05$. The evolution starts at $k = \Lambda \gg 1$ with $U_\Lambda = V$. It is apparent that for $k \gg 1$ the potential U_k changes very little. This means that the

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[1] We use $\hbar = 1$ throughout the paper.

ultraviolet (short-distance) fluctuations do not contribute to the evolution, and reflects the absence of ultraviolet divergences in quantum mechanics. For $k = \mathcal{O}(1)$ the evolution becomes fast, while the location of the minima moves to zero. Eventually, the evolution slows down for $k \to 0$ and the potential takes its final form with only one minimum at the origin.

Several properties of this solution have physical significance:

- In one dimension, the location of the minimum always runs to zero for $k \to 0$. This reflects the absence of spontaneous symmetry breaking in quantum mechanics.

- The value of the potential at the minimum changes from zero to a positive value. In more than one dimensions, the absolute scale of the potential is related to the cosmological constant and is very sensitive to the contribution from the ultraviolet fluctuations. In one dimension, the ultraviolet contributions are negligible and the absolute scale of the potential is meaningful. In fact, the value of $U_0 = U$ at the minimum corresponds to the expectation value of the system in the vacuum, i.e. the eignevalue E_0 of the ground state. In our case $E_0 = U(0)$.

- In field-theoretical terms, the first excitation of the system above the vacuum corresponds to a particle at rest. Its mass term is given by the second derivative of the potential with respect to ϕ at the minimum. This means that the eigenvalue of the first excited quantum-mechanical state can be computed as $E_1 = E_0 + \sqrt{\partial^2 U(0)/\partial \phi^2}$.

- If the lowest energy eigenvalue E_0 is below the maximum of the barrier of the classical potential $V(0) = 1/(16\lambda)$ (as in our example), tunnelling plays an important role in the problem. The solutions are then of trully non-perturbative nature.

In fig. 2 we plot $\left[\partial^2 U_k(\phi)/\partial \phi^2\right]/k^2$ during the whole evolution. The continuous lines depict the initial part of the running with $\Lambda \geq k \gtrsim 1$, while the dashed ones the final part with $1 \gtrsim k \geq 0$. We observe that there is a range of k for which $\partial^2 U_k(\phi)/\partial \phi^2 \simeq -k^2$ near the origin of the potential. The reason for this behaviour is the presence of a pole at -1 for $\left[\partial^2 U_k(\phi)/\partial \phi^2\right]/k^2$ in eq. (2). As this pole cannot be crossed, $\partial^2 U_k(\phi)/\partial \phi^2$ remains close to $-k^2$ while k is reduced towards zero. The pole is approached only for $\lambda \lesssim 0.1$ and the part of the evolution the system spends near it grows for $\lambda \to 0$. In this limit the importance of the barrier increases.

This behaviour has been observed in studies of field theories with spontaneous symmetry breaking in higher dimensions [12]. It results in the presence of a flat part of the potential between the two minima for $k \to 0$. ($\partial^2 U_{k \to 0}(\phi)/\partial \phi^2$ becomes zero between the minima.) It cannot be reproduced through the expansion of $U_k(\phi)$ in powers of ϕ employed in ref. [13]. In the one-dimensional case we are studying, the minimum of the potential always moves to the origin and $\partial^2 U_k(0)/\partial \phi^2$ becomes positive at the end of the evolution. However, the longer the part of the evolution the system spends near the pole, the smaller the final positive value of $\partial^2 U_{k \to 0}(0)/\partial \phi^2$. As this value determines the difference between the first two energy eigenvalues, the presence of the pole in the evolution equation predicts a vanishing $E_1 - E_0$ for $\lambda \to 0$. This is in qualitative agreement with the expectation from quantum mechanics.

The quantitative accuracy of the predictions can be checked through comparison with the results of the numerical solution of the Schrödinger equation with a potential given by eq. (3). In fig. 3 we plot the values of E_0, E_1 predicted by the solution of the evolution equation, along with the exact results, as a function of λ. We also show the height of the barrier $V(0) = 1/(16\lambda)$. Comparison with E_0, E_1 determines how important tunnelling is for the corresponding solutions. In fig. 4 we give values for the difference $\Delta E = E_1 - E_0$. We also include the prediction of the dilute-gas instanton

approximation [16, 13]

$$\Delta E = 2\sqrt{\frac{2\sqrt{2}}{\pi\lambda}} \exp\left(-\frac{1}{3\sqrt{2}\lambda}\right). \tag{4}$$

For $\lambda \gtrsim 0.15$ the agreement between the values of E_0 and E_1 resulting from our analysis and the exact results is at the few-per-cent level. For $\lambda = \mathcal{O}(1)$ it becomes better than 1%. The deviations are in the same direction, so that our prediction for the difference ΔE agrees at a level better than 1% with the exact value for all $\lambda \gtrsim 0.15$. We conclude that the lowest order of the derivative expansion (eq. (1)) leads to very good quantitative results when the potential does not have a large barrier. This conclusion is reaffirmed through the study of a potential without a barrier. In fig. 5 we give the results for the unharmonic oscillator, corresponding to the potential of eq. (3) with a mass term $m^2 = -1$. All this is in very good agreement with ref. [13], which indicates that the additional approximation of the potential by a polynomial, employed there, is very good for large λ.

For $\lambda \lesssim 0.15$ the lowest energy eigenvalue is below the top of the barrier of the classical potential. This means that tunnelling plays a significant role in the solution. In the region $0.09 \lesssim \lambda \lesssim 0.15$ our results have an accuracy better than 10%. We conclude that the renormalization group accounts reasonably well for tunnelling effects in this region. For $\lambda \lesssim 0.09$ the energy eigenvalue of the first excited state is below the top of the barrier as well. Our results have large deviations from the exact values and the renormalization-group approach fails to give a good quantitative picture. However, the correct qualitative behaviour is still reproduced. In fig. 4 we observe that the difference ΔE diminishes with decreasing λ. Excessive requirements in computer time, in order to reproduce correctly the solution near the pole, forbid the numerical integration of eq. (2) for very small λ. Already for $\lambda = 0.04$ the numerical error becomes close to 1%. However, as we explain below, we expect that ΔE becomes 0 for $\lambda \to 0$. An extrapolation of our results in this limit, as well as an approximate analytical solution (see below), verifies our expectation. However, the correct quantitative dependence of ΔE on λ, given by the dilute-gas instanton approximation (eq. (4)), is not reproduced.

Discussion: In order to understand better the nature of the solutions of the partial differential equation (2), it is useful to consider some approximations that permit an analytical treatment. For large k the potential has a minimum $\phi_0(k)$ away from the origin. The k-dependence of the minimum can be obtained by considering the total k-derivative of the condition $\partial U_k/\partial\phi|_{\phi=\phi_0} = 0$. One finds

$$\frac{d\phi_0}{dk} = -\frac{1}{U_k''(\phi_0)}\frac{\partial U_k'(\phi_0)}{\partial k} = \frac{1}{2\pi}\frac{U_k'''(\phi_0)}{U_k''(\phi_0)}\frac{1}{k^2}\left[1 + \frac{U_k''(\phi_0)}{k^2}\right]^{-1}, \tag{5}$$

where primes denote derivatives with respect to ϕ. For small λ the potential $U_k(\phi)$ can be approximated by a quartic polynomial, as in eq. (3). Moreover, the coefficient of the quartic term has a weak dependence on k, as can be verified through the numerical solution. Within perturbation theory, one can explain the smallness of the omitted corrections by the fact that they involve powers of λ.

We consider first the case in which $U_k''(\phi_0)/k^2 \ll 1$ during the whole evolution. Within our appoximations, eq. (5) can be integrated easily with the result

$$\phi_0^2(k) = \phi_0^2(\Lambda) - \frac{3}{\pi}\frac{1}{k}, \tag{6}$$

where we have assumed $\Lambda \gg 1$. For any initial $\phi_0(\Lambda)$ there is a value $k_{cr} = 3/(\pi\phi_0^2(\Lambda)) = 12\lambda/\pi$ at which the minimum moves to the origin. This is in agreement with our expectation that spontaneous

symmetry breaking cannot appear in one dimension. At scales below k_{cr} the minimum remains at the origin, while the mass term obeys the equation

$$\frac{dU_k''(0)}{dk} = -\frac{1}{2\pi} \frac{U_k^{(4)}(0)}{k^2} \left[1 + \frac{U_k''(0)}{k^2}\right]^{-1}.$$ (7)

For positive $U_k^{(4)}(0)$, the mass term grows as k is further reduced. The evolution stops for very small k, when $U_k''(0) \gg k^2$ (decoupling).

It is possible that $U_k''(\phi_0)/k^2 = \mathcal{O}(1)$ before the minimum of the potential moves to zero. In the approximation of a quartic potential with a constant quartic coefficient $\lambda \lesssim 0.1$, we have $U_k''(\phi_0)/k^2 \simeq 1$ for $k_p \simeq 1 > k_{cr}$. This complicates the analytical study of eq. (5). Moreover, it raises the possibility that, as k^2 is reduced below k_p^2, it may become much smaller than $U_k''(\phi_0)$ and the evolution may stop with the system in the phase with symmetry breaking. This scenario is never realized because of the presence of a pole at $\partial^2 U_k/\partial\phi^2 = -k^2$ in the evolution equation (2). This pole is approached first at the origin, where eq. (7) applies. The relevant behaviour was analysed in detail in ref. [12] for field theories in more than one dimensions, where symmetry breaking can occur. It was shown that the solution approaches the limit $k \to 0$ with $U_k''(0) \simeq -k^2$. The curvature at the origin vanishes for $k = 0$ and this leads to the convexity of the effective potential. Polynomial approximations of the potential, such as the one employed in ref. [13], cannot reproduce this behaviour and lead to the appearance of singularities at non-zero values of k.

Our numerical solution, depicted in figs. 1 and 2, reproduces the correct behaviour for $\lambda = 0.05$. The inner part of the potential becomes very flat as the pole is approached. At some stage the flatness approaches the minima and prevents the decoupling behaviour that would occur for $U_k''(\phi_0) \gg k^2$. Eventually the minimum moves to the origin and the system settles in the symmetric phase. Because of the induced flatness near the origin, the mass term $\partial^2 U_{k\to 0}(\phi)/\partial\phi^2$ that determines the energy difference $E_1 - E_0$ is very small. As this type of behaviour becomes more pronounced in the limit $\lambda \to 0$, we expect that $E_1 - E_0$ becomes zero in this limit.

The unsatisfactory aspect of our study is that the correct quantitative behaviour for $\lambda \to 0$ is not reproduced by the renormalization-group approach. This is apparent in fig. 4, where the energy difference $E_1 - E_0$ is depicted. This quantity approaches zero linearly with λ, instead of $\sim \exp\left[-1/\left(3\sqrt{2}\lambda\right)\right]$, as predicted by the dilute-gas instanton approximation. We conclude that the first order of the derivative expansion cannot account quantitatively for the non-local effects associated with tunnelling.

However, the use of an alternative method, such as an expansion around a saddle point, can remedy the situation. A very good example is provided by the study of tunnelling rates in three dimensions [11]. The renormalization group can be used for the integration of high frequency fluctuations (that may even induce radiative symmetry breaking), while an expansion around a saddle point (such as the scalar instanton or bounce) can account for tunnelling effects. The complementarity of the two methods guarantees the consistency of the calculation.

An approximate analytical solution: As a final confirmation of the previous discussion we present an approximate analytical solution of the evolution equation near the origin of the potential. By defining the quantities $\rho = \phi^2/2$, $\tilde{\rho} = k\rho$, $u_k(\tilde{\rho}) = U_k(\rho)/k$, $t = \log k$, we can write eq. (2) as

$$\frac{\partial u_k'(\tilde{\rho})}{\partial t} = -2u_k' - \tilde{\rho}\, u_k'' - \frac{1}{2\pi} \frac{3u_k'' + 2\tilde{\rho}\, u_k'''}{1 + u_k' + 2\tilde{\rho}\, u_k''}.$$ (8)

Primes on $u_k(\tilde{\rho})$ denote derivatives with respect to $\tilde{\rho}$. Near the origin of the potential ($\tilde{\rho} \simeq 0$) we can approximate the above equation by

$$\frac{\partial u'_k}{\partial t} + \left(\tilde{\rho} + \frac{3}{2\pi}\frac{1}{1+u'_k}\right)\frac{\partial u'_k}{\partial \tilde{\rho}} + 2u'_k = 0. \tag{9}$$

This is a first-order partial differential equation for $u_k(\tilde{\rho})$, which can be solved with the method of characteristics.

The most general solution is

$$\tilde{\rho}\sqrt{u'_k} + \frac{3}{2\pi}\tan^{-1}\sqrt{u'_k} = F\left(u'_k e^{2t}\right) \qquad \text{for} \;\; u'_k > 0$$

$$\tilde{\rho}\sqrt{-u'_k} + \frac{3}{4\pi}\log\left(\frac{1+\sqrt{-u'_k}}{1-\sqrt{-u'_k}}\right) = G\left(u'_k e^{2t}\right) \qquad \text{for} \;\; u'_k < 0. \tag{10}$$

The functions F and G are determined by the initial condition for the potential at $k = \Lambda$. For the choice of eq. (3) with $m^2 = 1$ we find

$$F(x) = \frac{1}{8\lambda}(1+x)\sqrt{x} + \frac{3}{2\pi}\tan^{-1}\left(\frac{\sqrt{x}}{\Lambda}\right)$$

$$G(x) = \frac{1}{8\lambda}(1+x)\sqrt{-x} + \frac{3}{4\pi}\log\left(\frac{1+\frac{\sqrt{-x}}{\Lambda}}{1-\frac{\sqrt{-x}}{\Lambda}}\right). \tag{11}$$

The above solution displays all the characteristic behaviour we discussed earlier. The minimum of the potential always moves to the origin at a scale $k_{cr} = 12\lambda/\pi$, while the pole at $k^{-2}\partial^2 U_k/\partial\phi^2 \simeq u'_k = -1$ is never crossed. We can also obtain an approximate expression for the mass term at the origin ($\tilde{\rho} = 0$) in the limit $k \to 0$, $u'_k(0) \to \infty$. We find $\sqrt{\partial U_{k\to 0}(0)/\partial\rho} = \sqrt{\partial^2 U_{k\to 0}(0)/\partial\phi^2} \simeq 6\lambda$, for small λ. This explains the linear dependence of ΔE on λ, observed in fig. 4 for small λ, even though the predicted slope is not quantitatively correct.

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Figures

- Fig. 1: The evolution of the potential as the coarse-graining scale is lowered from $k = \Lambda \gg 1$ to $k = 0$. The initial form of the potential is given by eq. (3) with $m^2 = 1$ and $\lambda = 0.05$.

- Fig. 2: Same as in fig. 1 for $\left[\partial^2 U_k / \partial \phi^2 \right] / k^2$.

- Fig. 3: The first two energy eigenvalues E_0, E_1, as predicted by the exact renormalization group in the lowest order of the derivative expansion, along with the exact results, as a function of λ, for the potential of eq. (3) with $m^2 = 1$. The dotted line indicates the height of the barrier for the potential of eq. (3).

- Fig. 4: The energy gap $E_1 - E_0$ as a function of λ. We display the exact values, the predictions of the exact renormalization group in the lowest order of the derivative expansion, and the results of the dilute-gas instanton approximation.
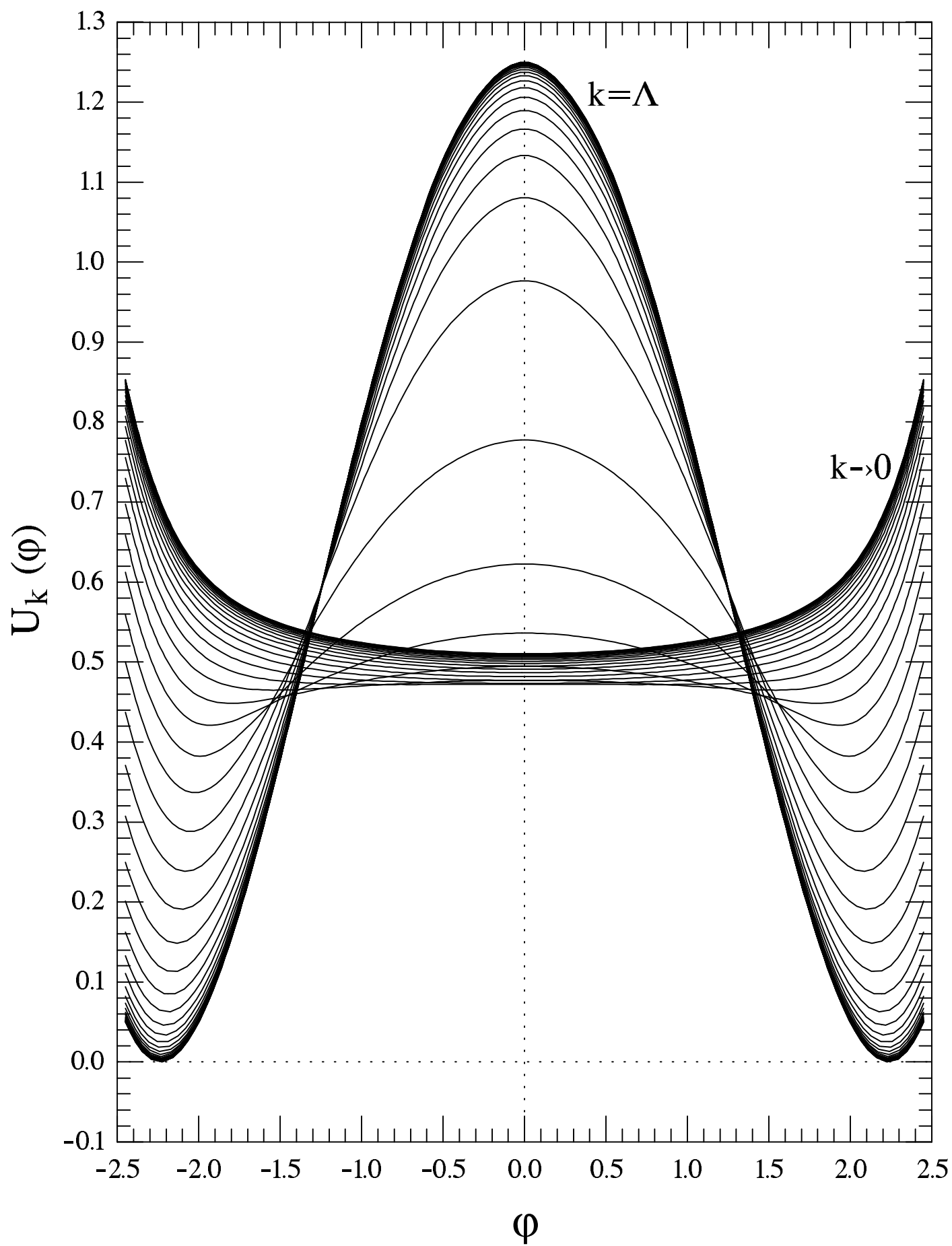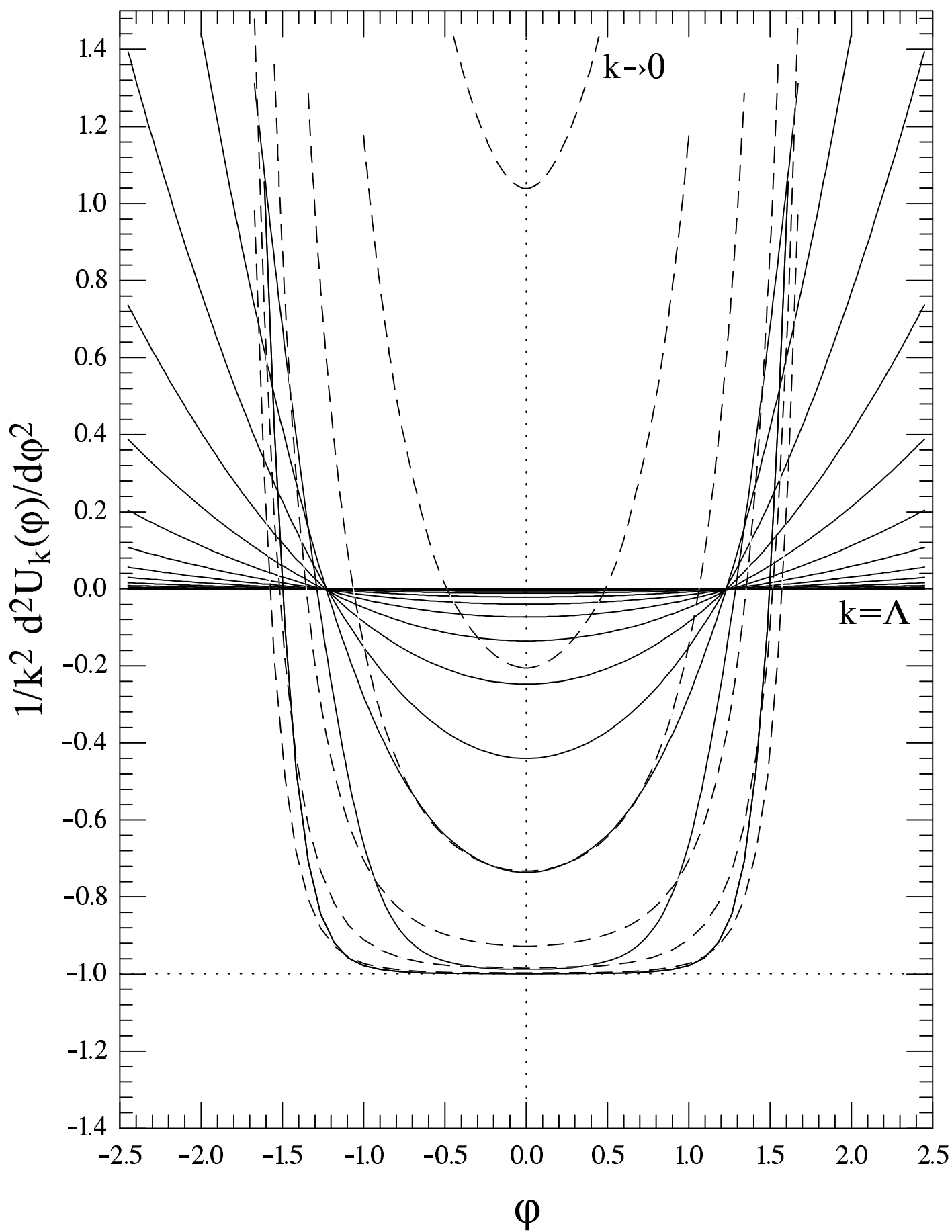
- Fig. 5: Same as in fig. 3 for the potential of eq. (3) with $m^2 = -1$.
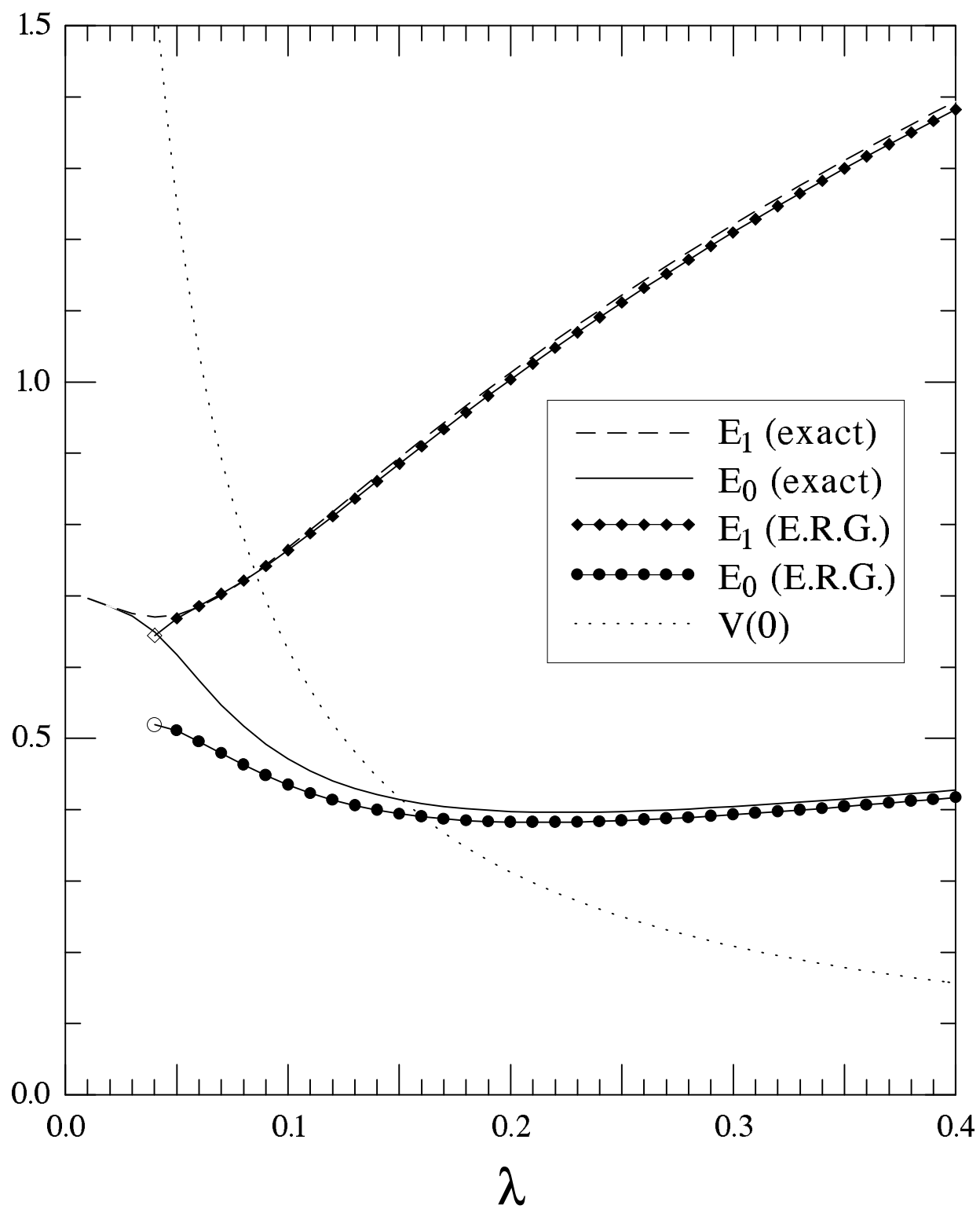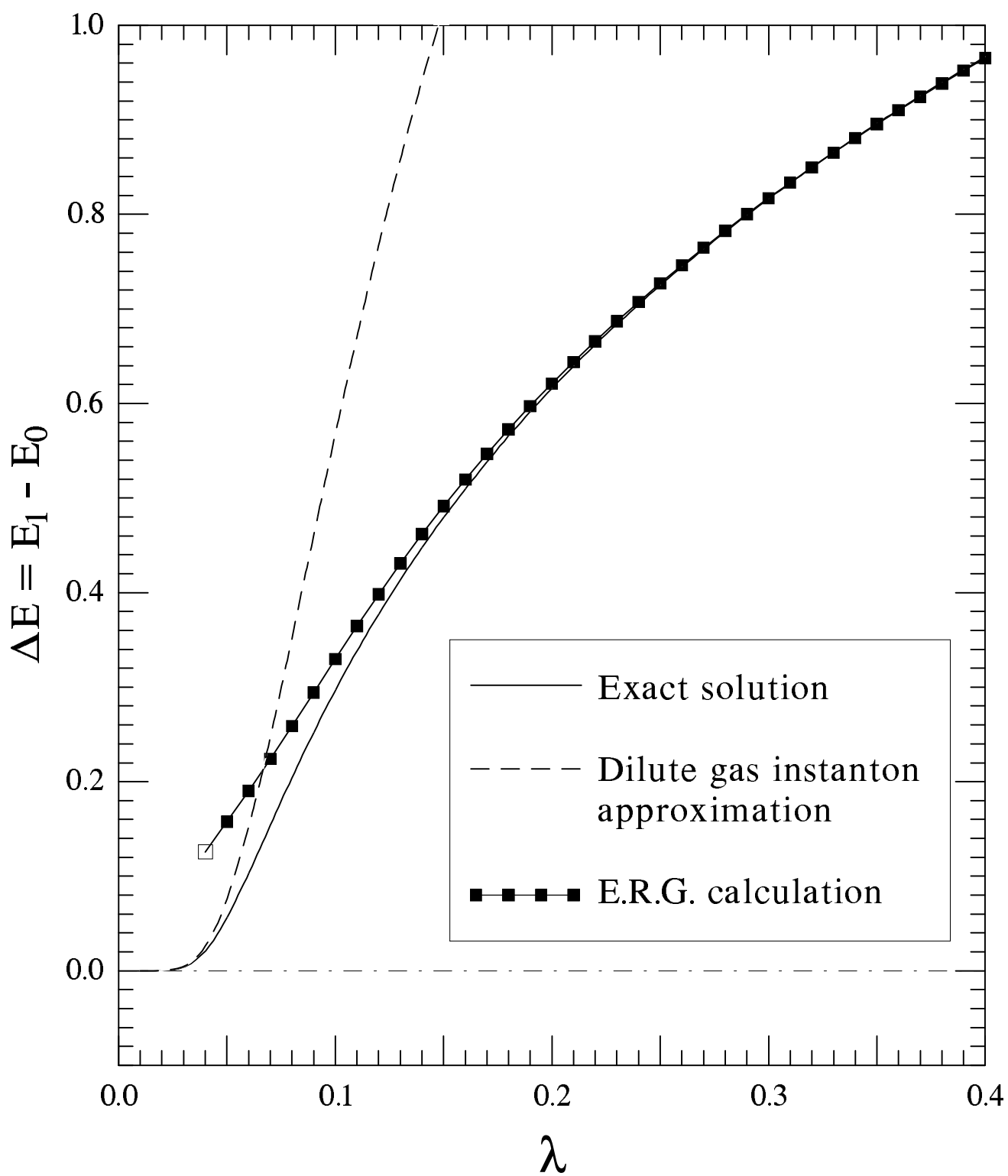
k=Λ

k→0

Fig. 1

Fig. 2

Fig. 3

Fig.4

Fig. 5